About Two Disinherited Sides of Statistics: Data Units and Computational Saving

Christophe Biernacki, Alexandre Lourme, Maxime Brunin, Alain A. Celisse

About Two Disinherited Sides of Statistics: Data Units and Computational Saving

C. Biernacki

8th ed. of the STATLEARN workshop "Challenging problems in Statistical Learning"
April 6-7, 2017, Lyon (France)

Synopsis of the talk

$$\widehat{\text{target}} \;=\; \mathbf{f}(\underbrace{\text{data}}_{\text{Part I}}, \text{model}, \underbrace{\text{algo}}_{\text{Part II}})$$

Part I

Unifying Data Units and Models in Statistics

Focus on (Co)-Clustering

Joint work with A. Lourme
(Bordeaux University)

Quizz!

$$y = \beta x^2 + e$$

- Is it a linear regression on co-variates (x^2)?
- Is it a quadratic regression on co-variates x?

Both!

Take home message

Units are entirely interrelated with models

This part:

- Be aware that interpretation of ("classical") models is unit dependent
- Models should even be revisited as a couple units $\times$ "classical" models
- Opportunity for cheap/wide/meaningful enlarging of "classical" model families
- Focus on model-based (co-)clustering but larger potential impact

General (model-based) statistical framework

- Data:
  - Whole data set composed by n objects, described by d variables

$$\mathbf{x} = (\mathbf{x}_1, \ldots, \mathbf{x}_n) \quad \text{with} \quad \mathbf{x}_i = (x_{i1}, \ldots, x_{id}) \in \mathbb{X}$$

  - Each $\mathbf{x}_i$ value is provided with a unit **id**
  - We note "**id**" since units are often user defined (a kind of canonical units)
- Model:
  - A pdf[1] family, indexed by $\mathbf{m} \in \mathbb{M}$[2]

$$\mathrm{p}_{\mathbf{m}} = \{\cdot \in \mathbb{X} \mapsto \mathrm{p}(\cdot; \boldsymbol{\theta}) : \boldsymbol{\theta} \in \Theta_{\mathbf{m}}\}$$

  - With $\mathrm{p}(\cdot; \boldsymbol{\theta})$ a (parametric) pdf and $\Theta_{\mathbf{m}}$ a space where evolves this parameter
- Target:

$$\widehat{\text{target}} = \mathbf{f}(\mathbf{x}, \mathrm{p}_{\mathbf{m}})$$

Unit **id** is hidden everywhere and could have consequences on the target estimation!

[1] probability density function

[2] Often, the index **m** is confounded with the distribution family itself as a shortcut

Changing the data units

- Principle of data units transformation $\mathbf{u}$:

$$\begin{array}{llll} \mathbf{u}: & \mathbb{X} = \mathbb{X}^{\mathbf{id}} & \longrightarrow & \mathbb{X}^{\mathbf{u}} \\ & \mathbf{x} = \mathbf{x}^{\mathbf{id}} = \mathbf{id}(\mathbf{x}) & \longmapsto & \mathbf{x}^{\mathbf{u}} = \mathbf{u}(\mathbf{x}) \end{array}$$

- $\mathbf{u}$ is a bijective mapping to preserve the whole data set information quantity
- We denote by $\mathbf{u}^{-1}$ the reciprocal of $\mathbf{u}$, so $\mathbf{u}^{-1} \circ \mathbf{u} = \mathbf{id}$
- Thus, $\mathbf{id}$ is only a particular unit $\mathbf{u}$
- Often a meaningful restriction[3] on $\mathbf{u}$: it proceeds lines by lines and rows by rows

$$\mathbf{u}(\mathbf{x}) = (\mathbf{u}(\mathbf{x}_1), \ldots, \mathbf{u}(\mathbf{x}_n)) \quad \text{with} \quad \mathbf{u}(\mathbf{x}_i) = (\mathbf{u}_1(x_{i1}), \ldots, \mathbf{u}_d(x_{id}))$$

  - Advantage to respect the variable definition, transforming only its unit
  - $\mathbf{u}(\mathbf{x}_i)$ means that $\mathbf{u}$ applied to the data set $\mathbf{x}_i$, restricted to the single individual i
  - $\mathbf{u}_j$ corresponds to the specific (bijective) transformation unit associated to variable j

[3] Possibility to relax this restriction, including for instance linear transformations involved in PCA (principal component analysis). But the variable definition is no longer respected.

Revisiting units as a modelling component

- Explicitly exhibiting the "canonical" unit **id** in the model

$$p_{\mathbf{m}} = \{\cdot \in \mathbb{X} \mapsto p(\cdot;\boldsymbol{\theta}) : \boldsymbol{\theta} \in \Theta_{\mathbf{m}}\} = \{\cdot \in \mathbb{X}^{\mathbf{id}} \mapsto p(\cdot;\boldsymbol{\theta}) : \boldsymbol{\theta} \in \Theta_{\mathbf{m}}\} = p_{\mathbf{m}}^{\mathbf{id}}$$

- Thus the variable space and the probability measure are embedded
- As the standard probability theory: a couple (variable space,probability measure)!
- Changing **id** into **u**, while preserving **m**, is expected to produce a new modelling

$$p_{\mathbf{m}}^{\mathbf{u}} = \{\cdot \in \mathbb{X}^{\mathbf{u}} \mapsto p(\cdot;\boldsymbol{\theta}) : \boldsymbol{\theta} \in \Theta_{\mathbf{m}}\}.$$

A model should be systematically defined by a couple (**u**,**m**), denoted by $p_{\mathbf{m}}^{\mathbf{u}}$

Interpretation and identifiability of $p^{\mathbf{u}}_{\mathbf{m}}$

- Standard probability theory (again): there exists a measure $\mathbf{u}^{-1}(\mathbf{m})$ s.t.[4]

$$\mathbf{u}^{-1}(\mathbf{m}) \in \{\mathbf{m}' \in \mathbb{M} : p^{\mathbf{id}}_{\mathbf{m}'} = p^{\mathbf{u}}_{\mathbf{m}}\}$$

- There exists two alternative interpretations of strictly the same model:
  - $p^{\mathbf{u}}_{\mathbf{m}}$: data measured with unit $\mathbf{u}$ arise from measure $\mathbf{m}$;
  - $p^{\mathbf{id}}_{\mathbf{u}^{-1}(\mathbf{m})}$: data measured with unit $\mathbf{id}$ arise from measure $\mathbf{u}^{-1}(\mathbf{m})$
- Two points of view:

Statistician

The model $p^{\mathbf{u}}_{\mathbf{m}}$ is not identifiable over the couple $(\mathbf{m}, \mathbf{u})$

Practitioner

Freedom to choose the interpretation which is the most meaningful for him

[4] This set is usually restricted to a single element

Opportunity for designing new models

Great opportunity to build easily numerous new meaningful models $p_{\mathbf{m}}^{\mathbf{u}}$!

- Just combine a standard model family $\{\mathbf{m}\}$ with a standard unit family $\{\mathbf{u}\}$
- New family can be huge! Combinatorial problems can occur. . .
- Some model stability can exist in some (specific) cases: $\mathbf{m} = \mathbf{u}^{-1}(\mathbf{m})$

Model selection

As any model, possible to choose between $p^{\mathbf{u}_1}_{\mathbf{m}_1}$ and $p^{\mathbf{u}_2}_{\mathbf{m}_2}$

However, caution when using likelihood-based model selection criteria (as BIC)

- Prohibited to compare $\mathbf{m}_1$ in unit $\mathbf{u}_1$ and $\mathbf{m}_2$ in unit $\mathbf{u}_2$
- But allowed after transforming in identical unit **id**
- Thus compare their equivalent expression: $p^{\mathbf{id}}_{\mathbf{u}_1^{-1}(\mathbf{m}_1)}$ and $p^{\mathbf{id}}_{\mathbf{u}_2^{-1}(\mathbf{m}_2)}$
- Example for abs. continuous $\mathbf{x}$ and differentiable $\mathbf{u}$, the density transform in **id** is:

$$p^{\mathbf{id}}_{\mathbf{u}^{-1}(\mathbf{m})} = \{\cdot \in \mathbb{X}^{\mathbf{id}} \mapsto p(\mathbf{u}(\cdot);\boldsymbol{\theta}) \times |\mathbf{J}^{\mathbf{u}}(\cdot)| : \boldsymbol{\theta} \in \Theta_{\mathbf{m}}\}$$

with $\mathbf{J}^{\mathbf{u}}(\cdot)$ the Jacobian associated to the transformation $\mathbf{u}$

Focus on the clustering target

A current challenge is to enlarge model collection. . . and units could contribute to it!

- Model: mixture model $\mathbf{m}$ of parameter $\boldsymbol{\theta} = \{\pi_k, \boldsymbol{\alpha}_k\}_{k=1}^{g}$

$$\mathrm{p}_{\mathbf{m}}(\boldsymbol{x}; \boldsymbol{\theta}) = \sum_{k=1}^{g} \pi_k \mathrm{p}(\boldsymbol{x}; \boldsymbol{\alpha}_k)$$

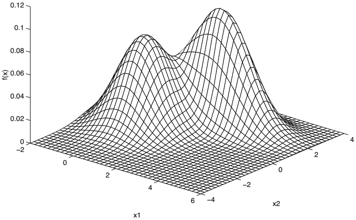
  - g is the number of clusters
  - Clusters correspond to a hidden partition $\mathbf{z} = (z_1, \ldots, z_n)$, where $z_i \in \{1, \ldots, g\}$
  - $\pi_k = \mathrm{p}(Z = k)$ and $\mathrm{p}(\boldsymbol{x}; \boldsymbol{\alpha}_k) = \mathrm{p}(\boldsymbol{X} = \mathbf{x} | Z = k)$
- Target: estimate $\mathbf{z}$ (and often g)
  - Estimate $\hat{\boldsymbol{\theta}}_{\mathbf{m}}$ by maximum likelihood (typically)
  - Estimate $\mathbf{z}$ by the MAP principle $\hat{z}_i = \arg\max_{k \in \{1,\ldots,g\}} \mathrm{p}(Z_i = k | \boldsymbol{X}_i = \mathbf{x}_i; \hat{\boldsymbol{\theta}}_{\mathbf{m}})$
  - Estimate g by BIC or ICL criteria typically (maximum likelihood based criteria)

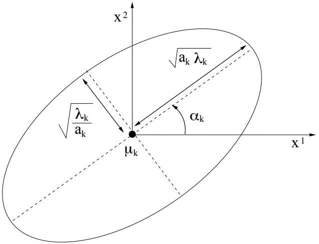
Outline

14 spectral models on $\boldsymbol{\Sigma}_k$

- $\mathbb{X} = \mathbb{R}^d$
- d-variate Gaussian model $\mathbf{m}$: $p_{\mathbf{m}}(\cdot; \boldsymbol{\alpha}_k) = \mathcal{N}_d(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$
- [Celeux & Govaert, 1995][5] propose the following eigen decomposition

$$\boldsymbol{\Sigma}_k = \underbrace{\lambda_k}_{\text{volume}} \cdot \underbrace{\mathbf{D}_k}_{\text{orientation}} \cdot \underbrace{\boldsymbol{\Lambda}_k}_{\text{shape}} \cdot \mathbf{D}_k'$$





[5] Celeux, G., and Govaert, G.. Gaussian parsimonious clustering models. Pattern Recognition, 28(5), 781–793 (1995).

Scale unit invariance

- Consider scale unit transformation $\mathbf{u}(\mathbf{x}) = \mathbf{D}\mathbf{x}$, with diagonal $\mathbf{D} \in \mathbb{R}^{d \times d}$
- Very current transformation: standard units (mm, cm), standardized units
- [Biernacki & Lourme, 2014] listed models where invariance holds (8 among 14)
  - The general model is invariant:

$$[\lambda_k \boldsymbol{S}_k \boldsymbol{\Lambda}_k \boldsymbol{S}_k'] = \mathbf{u}^{-1}([\lambda_k \boldsymbol{S}_k \boldsymbol{\Lambda}_k \boldsymbol{S}_k'])$$

  - An example of not invariant model:

$$[\lambda_k \boldsymbol{S} \boldsymbol{\Lambda}_k \boldsymbol{S}'] \neq \mathbf{u}^{-1}([\lambda_k \boldsymbol{S} \boldsymbol{\Lambda}_k \boldsymbol{S}'])$$

- Do not forget to compare all models $\mathbf{m}' = \mathbf{u}^{-1}(\mathbf{m})$ in unit **id** for BIC / ICL validity
- Use the `Rmixmod` package

Illustration on the Old Faithful geyser data set

- All models are with free proportions (π_k)
- All ICL values are expressed with the initial unit **id**=min×min
- We observe the effect of unit on the ICL ranking for some models
- Cheap opportunity to enlarge the model family!

	$\mathbf{id}$ = (min, min)		$\mathbf{u}^{\text{scale}_1}$ = (sec, min)		$\mathbf{u}^{\text{scale}_2}$ = (stand, stand)	
family	**m**	$\text{ICL}^{\mathbf{id}}$	**m**	$\text{ICL}^{\mathbf{id}}$	**m**	$\text{ICL}^{\mathbf{id}}$
All mod.	$[\lambda_k \boldsymbol{S} \boldsymbol{\Lambda}_k \boldsymbol{S}']$	1 160.3	$[\lambda_k \boldsymbol{S} \boldsymbol{\Lambda}_k \boldsymbol{S}']$	1 158.7	$[\lambda_k \boldsymbol{S}_k \boldsymbol{\Lambda} \boldsymbol{S}_k']$	1 160.3
General mod.	$[\lambda_k \boldsymbol{S}_k \boldsymbol{\Lambda}_k \boldsymbol{S}_k']$	1 161.4	$[\lambda_k \boldsymbol{S}_k \boldsymbol{\Lambda}_k \boldsymbol{S}_k']$	1 161.4	$[\lambda_k \boldsymbol{S}_k \boldsymbol{\Lambda}_k \boldsymbol{S}_k']$	1 161.4

Outline

Prostate cancer data of [Biar & Green, 1980][8]

- Individuals: 506 patients with prostatic cancer grouped on clinical criteria into two Stages 3 and 4 of the disease
- Variables: $d = 12$ pre-trial variates were measured on each patient, composed by
  - Eight continuous variables (age, weight, systolic blood pressure, diastolic blood pressure, serum haemoglobin, size of primary tumour "SZ", index of tumour stage and histolic grade, serum prostatic acid phosphatase "AP")
  - Two ordinal variables (performance rating, cardiovascular disease history)
  - Two categorical variables with various numbers of levels (electrocardiogram code, bone metastases)
- Some missing data: 62 missing values ($\approx 1\%$)
- Two historical units for performing the clustering task:
  - Raw units **id**: [McParland & Gormley, 2015][6]
  - Transformed data **u**: since SZ and AP are skewed, [Jorgensen & Hunt, 1996][7] propose

$$\mathbf{u}_{SZ} = \sqrt{\cdot} \text{ and } \mathbf{u}_{AP} = \ln(\cdot)$$

[6] McParland, D. and Gormley, I. C. (2015). Model based clustering for mixed data: clustmd. arXiv preprint arXiv:1511.01720.

[7] Jorgensen, M. and Hunt, L. (1996). Mixture model clustering of data sets with categorical and continuous variables. In Proceedings of the Conference ISIS, volume 96, pages 375–384.

[8] Byar DP, Green SB (1980): Bulletin Cancer, Paris 67:477-488

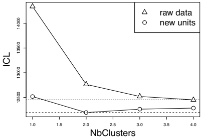
Clustering with the MixtComp software [Biernacki *et al.*, 2016][9]

- Model $\mathbf{m}$ in Mixtcomp: full mixed data $\mathbf{x} = (\mathbf{x}^{cont}, \mathbf{x}^{cat}, \mathbf{x}^{ordi}, \mathbf{x}^{int}, \mathbf{x}^{rank})$ (missing data are allowed also) are simply modeled by inter conditional independence

$$p(\mathbf{x}; \boldsymbol{\alpha}_k) = p(\mathbf{x}^{cont}; \boldsymbol{\alpha}_k^{cont}) \times p(\mathbf{x}^{cat}; \boldsymbol{\alpha}_k^{cat}) \times p(\mathbf{x}^{ordi}; \boldsymbol{\alpha}_k^{ordi}) \times \dots$$

  In addition, for symmetry between types, intra conditional independence for each

- Results:
  - New units $\mathbf{u}_{SZ}$ and $\mathbf{u}_{AP}$ are selected by ICL
  - New units allow to select two groups and provides a lower error rate



clusters	
1	2
287	5
52	162

Table : MixtComp model on raw units: 11% misclassified

clusters	
1	2
270	22
23	191

Table : MixtComp model on new units: 9% misclassified

[9] MixtComp is a clustering software developped by Biernacki C., Iovleff I. and Kubicki V. and freely available on the MASSICCC web platform https://massiccc.lille.inria.fr/

Outline

Which units for count data?

- Count data: $x \in \mathbb{N}$
- Standard model $\mathbf{m}$ is Poisson: $\mathrm{p}(\cdot; \alpha_k) = \mathcal{P}(\lambda_k)$
- d-variate case $\mathbf{x} = (x^1, \ldots, x^d) \in \mathbb{N}^d$ and conditional independence by variable
- Two standards unit transformations (by variable $j \in \{1, \ldots, d\}$):
  - Shifted observations: $\mathbf{u}(x^j) = x^j - a_j$ with $a_j \in \mathbb{N}$
  - Scaled observations: $\mathbf{u}(x^j) = b_j x^j$ with $b_j \in \mathbb{N}^*$

Shifted example

- **id**: total number of educational years
- $\mathbf{u}_{shift}(\cdot) = (\cdot) - 8$: university number of educational years[a]

[a] Eight is the number of years spent by english pupils in a secondary school.

Scaled example

- **id**: total number of educational years
- $\mathbf{u}_{scaled}(\cdot) = 2 \times (\cdot)$: total number of educational semesters

Medical data

- R dataset `rwm1984COUNT` of [Rao *et al.*, 2007, p.221][10] and studied in [Hilbe, 2014][11]
- $n = 3874$ patients that spent time into German hospitals during year 1984
- Patients are described through eleven mixed variables
- **m**: a MixtComp model combining Gaussian, Poisson and multinomial distributions

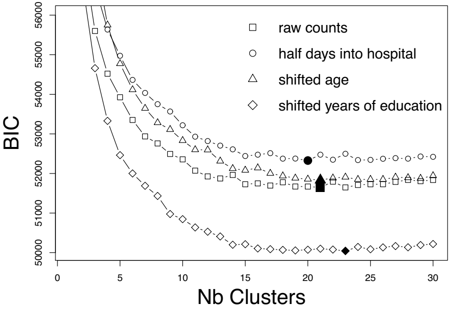
	variables	*type*	*model*
1	number of visits to doctor during year	count	Poisson
2	number of days in hospital	count	Poisson
3	educational level	categorical	multinomial
4	age	count	Poisson
5	outwork	binary	Bernoulli
6	gender	binary	Bernoulli
7	matrimonial status	binary	Bernoulli
8	kids	binary	Bernoulli
9	household yearly income	continous	Gaussian
10	years of education	count	Poisson
11	self employed	binary	Bernoulli

[10] Rao, C. R., Miller, J. P., and Rao, D. C. (2007). Handbook of statistics: epidemiology and medical statistics, volume 27. Elsevier.

[11] Hilbe, J. M. (2014). Modeling count data. Cambridge University Press.

Several units for count data

- Four unit systems are sequentially considered differing over the count data
  - $\mathbf{u}_1 = \mathbf{id}$: original unit
  - $\mathbf{u}_2$: the time spent into hospital is counted in half days instead of days
  - $\mathbf{u}_3$: the minimum of the age series is deduced from all ages leading to shifted ages
  - $\mathbf{u}_4$: the min. of years of edu. is deduced from the series leading to shifted years of edu.
- BIC selects 23 clusters obtained under shifted years of education



Specific transformation for RNA-seq data

- A sample of RNA-seq gene expressions arising from the rat count table of `http://bowtie-bio.sourceforge.net/recount/`
- 30000 genes described by 22 counting descriptors
- Remove genes with low expression (classical): 6173 genes finally
- Two different processes for dealing with data:
  - Standard [Rau *et al.*, 2015][12]: $\mathbf{u} = \mathbf{id}$ and $\mathbf{m}$ is Poisson mixture
  - "RNA-seq unit" [Gallopin *et al.*, 2015][13]:

$$\mathbf{u}(\cdot) = \ln(\text{scaled normalization}(\cdot))$$

  is a transformation being motivated by genetic considerations and $\mathbf{m}$ is Gaussian mixture
  - Experiment with 30 clusters (as in [Gallopin *et al.*, 2015])

model	*data*	*BIC*
Poisson	raw unit	2 615 654
Gaussian	transformed	909 190

[12] Rau, A., Maugis-Rabusseau, C. , Martin-Magniette, M.-L. and Celeux, G. (2015). Co-expression analysis of high-throughput transcriptome sequencing data with Poisson mixture models. Bioinformatics, 31 (9), 1420-1427.

[13] Gallopin, M., Rau, A., Celeux, G., and Jaffrézic, F. (2015). Transformation des données et comparaison de modèles pour la classification des données rna-seq. In 47èmes Journées de Statistique de la SFdS.

Outline

Co-clustering framework

- It corresponds to the following specific mixture model $\mathbf{m}$ [Govaert and Nadif, 2014][14]:

$$\mathrm{p}(\mathbf{x};\boldsymbol{\theta}) = \sum_{(\mathbf{z},\mathbf{w})} \prod_{i,j} \pi_{z_i}\rho_{w_j}\mathrm{p}(x_i^j;\boldsymbol{\alpha}_{z_i w_j})$$

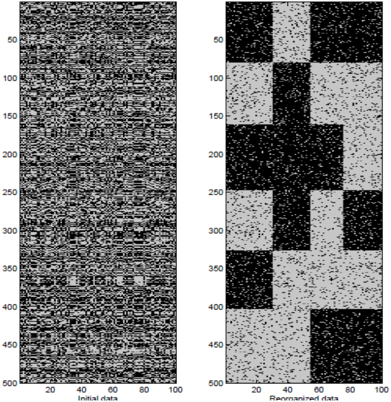
  - $\mathbf{z}$: partition in g_r rows
  - $\mathbf{w}$: partition in g_c columns
  - $\mathbf{z} \perp \mathbf{w}$ and $x_i^j|(z_i, w_j) \perp x_{i'}^{j'}|(z_{i'}, w_{j'})$
- Distribution $\mathrm{p}(\cdot;\boldsymbol{\alpha}_{z_i w_j})$ depends on the kind of data
  - Binary data: $x_i^j \in \{0,1\}$, $\mathrm{p}(\cdot;\boldsymbol{\alpha}_{kl}) = \mathcal{B}(\alpha_{kl})$
  - Categorical data with m levels:
    $\mathbf{x}_i^j = \{x_i^{jh}\} \in \{0,1\}^m$ with $\sum_{h=1}^m x_i^{jh} = 1$ and $\mathrm{p}(\cdot;\boldsymbol{\alpha}_{kl}) = \mathcal{M}(\boldsymbol{\alpha}_{kl})$ with $\boldsymbol{\alpha}_{kl} = \{\alpha_k^{jh}\}$
  - Count data: $x_i^j \in \mathbb{N}$, $\mathrm{p}(\cdot;\boldsymbol{\alpha}_{kl}) = \mathcal{P}(\mu_k\nu_l\gamma_{kl})$
  - Continuous data: $x_i^j \in \mathbb{R}$, $\mathrm{p}(\cdot;\boldsymbol{\alpha}_{kl}) = \mathcal{N}(\mu_{kl}, \sigma_{kl}^2)$
- `BlockCluster` [Bhatia *et al.*, 2015][15] is an R package for co-clustering

---

[14] G. Govaert and M. Nadif (2014). Co-clustering: models, algorithms and applications. ISTE, Wiley. ISBN 978-1-84821-473-6.

[15] P. Bhatia, S. Iovleff, G. Govaert (2015). Blockcluster: An R Package for Model Based Co-Clustering. *Journal of Statistical Software*, in press.

Binary illustration



Outline

SPAM E-mail Database[17]

- $n = 4601$ e-mails composed by 1813 "spams" and 2788 "good e-mails"
- $d = 48 + 6 = 54$ continuous descriptors[16]
  - 48 percentages that a given word appears in an e-mail ("make", "you'...)
  - 6 percentages that a given char appears in an e-mail (";", "$"...)
- Transformation of continuous descriptors into binary descriptors

$$x_i^j = \begin{cases} 1 & \text{if word/char } j \text{ appears in e-mail } i \\ 0 & \text{otherwise} \end{cases}$$

Two different units considered for variable $j \in \{1, \ldots, 54\}$

- $\mathbf{id}_j$: see the previous coding
- $\mathbf{u}_j(\cdot) = 1 - (\cdot)$: reverse the coding

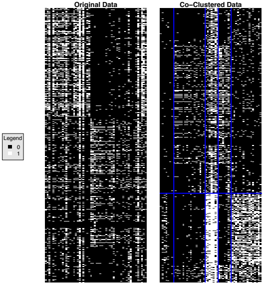
$$\mathbf{u}_j(x_i^j) = \begin{cases} 0 & \text{if word/char } j \text{ appears in e-mail } i \\ 1 & \text{otherwise} \end{cases}$$

[16] There are 3 other continuous descriptors we do not use

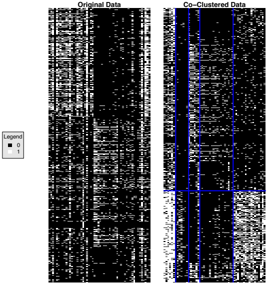
[17] https://archive.ics.uci.edu/ml/machine-learning-databases/spambase/

Select the whole coding $\mathbf{u} = (\mathbf{u}_1, \ldots, \mathbf{u}_d)$

- Fix $g_l = 2$ (two individual classes) and $g_r = 5$ (five variable classes)
- Use co-clustering in a clustering aim: just interested in indiv. classes (spams?)
- Use a "naive" algorithm to find the best $\mathbf{u}$ by ICL (2^{54} possibilities)



initial unit **id**
ICL=92682.54
error rate=0.1984



best unit $\mathbf{u}$
ICL=92524.57
error rate=0.2008

Result analysis of the e-mail database

- Just one variable ($j = 19$: "you") has a reversed coding in $\mathbf{u}$
- Thus variable "you" has not the same coding as other variables in its column class
- Poor ICL increase with $\mathbf{u}$

Conclusion for the e-mail database

- Here initial units **id** have a particular meaning for the user: do not change!
- In case of unit change, it becomes essentially technic (as Manly unit is)

Outline

Congressional Voting Records Data Set[19]

- Votes for each of the $n = 435$ U.S. House of Representatives Congressmen
- Two classes: 267 democrats, 168 republicans
- $d = 16$ votes with $m = 3$ modalities [Schlimmer, 1987][18]:
  - "yea": voted for, paired for, and announced for
  - "nay": voted against, paired against, and announced against
  - "?": voted present, voted present to avoid conflict of interest, and did not vote or otherwise make a position known

1. handicapped-infants
2. water-project-cost-sharing
3. adoption-of-the-budget-resolution
4. physician-fee-freeze
5. el-salvador-aid
6. religious-groups-in-schools
7. anti-satellite-test-ban
8. aid-to-nicaraguan-contras
9. mx-missile
10. immigration
11. synfuels-corporation-cutback
12. education-spending
13. superfund-right-to-sue
14. crime
15. duty-free-exports
16. export-administration-act-south-africa

[18] Schlimmer, J. C. (1987). Concept acquisition through representational adjustment. Doctoral dissertation, Department of Information and Computer Science, University of California, Irvine, CA.

[19] http://archive.ics.uci.edu/ml/datasets/Congressional+Voting+Records

Allowed user meaningful recodings

- "yea" and "nea" are arbitrarily coded (question dependent), not "?"
- Example:

3. adoption-of-the-budget-resolution = "yes" ⇔ 3. rejection-of-the-budget-resolution = "no"

- However, "?" is not question dependent

Thus, two different units considered for variable $j \in \{1, \ldots, 16\}$

- $\mathbf{id}_j$:

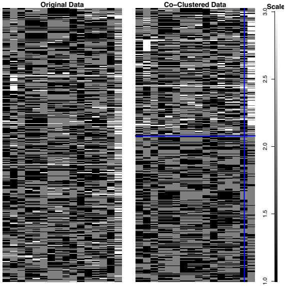
$$x_i^j = \begin{cases} (1,0,0) & \text{if voted "yea" to vote } j \text{ by congressman } i \\ (0,1,0) & \text{if voted "nay" to vote } j \text{ by congressman } i \\ (0,0,1) & \text{if voted "?" to vote } j \text{ by congressman } i \end{cases}$$

- $\mathbf{u} = (\mathbf{u}_1, \ldots, \mathbf{u}_d)$: reverse the coding only for "yea" and "nea"

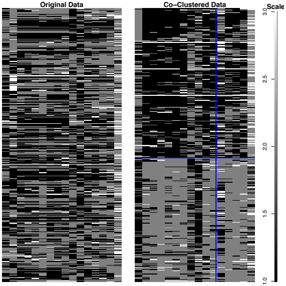
$$\mathbf{u}_j(x_i^j) = \begin{cases} (0,1,0) & \text{if voted "yea" to vote } j \text{ by congressman } i \\ (1,0,0) & \text{if voted "nay" to vote } j \text{ by congressman } i \\ (0,0,1) & \text{if voted "?" to vote } j \text{ by congressman } i \end{cases}$$

Select the whole coding $\mathbf{u} = (\mathbf{u}_1, \ldots, \mathbf{u}_d)$

- Fix $g_l = 2$ (two individual classes) and $g_r = 2$ (two variable classes)
- Use co-clustering in a clustering aim: just interested in political party
- Use a comprehensive algorithm to find the best $\mathbf{u}$ by ICL ($2^{16} = 65536$ cases)



initial unit **id**
ICL=5916.13
error rate=0.2850



best unit **u**
ICL=5458.156
error rate=0.1034

Result analysis of the Congressional Voting Records Data Set

- Five variables has a reversed coding in **u**:
  - 3. adoption-of-the-budget-resolution
  - 7. anti-satellite-test-ban
  - 9. aid-to-nicaraguan-contras
  - 10. mx-missile
  - 16. duty-free-exports
- Thus be aware to change the meaning of them when having a look at the figure!
- Significant ICL and error rate improvements with **u**

Conclusion for the Congressional Voting Records

- Here initial units **id** where arbitrary fixed: make sense to change!
- In addition, good improvement. . .

Part II

Computation Time/Accuracy Trade-off

Focus on Linear Regression

Joint work with M. Brunin & A. Célisse
(Lille University & CNRS & Inria)

An unexpected behaviour. . .

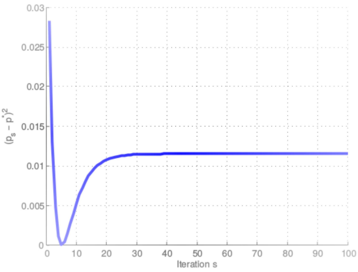
Standard idea

The larger is the iteration number, the better is the resulting estimate

Not so certain. . .

An early stopping rule could reduce computation time while increasing accuracy

Ex.: two Gaussian univariate mixture, just proportions unknown (convex), use EM



Take home message

Early stopping of some estimation algorithms could be statistically efficient while preserving computational time

This part:

- Identify bias/variance influence throughout the algorithm iterations
- Define an early stopping rule reaching the bias/variance trade-off
- Focus on linear regression but expected to be (much) more general

Outline

Linear regression

- Usual linear regression model:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\theta}^* + \boldsymbol{\epsilon},$$

with $\mathbf{X} \in \mathcal{M}_{n,d}(\mathbb{R})$, $\mathrm{rg}(\mathbf{X}) = d$ $(n > d)$, $\boldsymbol{\theta}^* \in \mathbb{R}^d$, $\boldsymbol{\epsilon} \sim \mathcal{N}_n\left(\mathbf{0}, \sigma^2 \mathbf{I}_n\right)$

- Usual Ordinary Least Squares (OLS) parameter estimate:

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}\in\mathbb{R}^d} \underbrace{\frac{1}{2n}\|\mathbf{Y} - \mathbf{X}\boldsymbol{\theta}\|_{2,n}^2}_{g(\boldsymbol{\theta})} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$

- Usual OLS prediction estimate:

$$\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\theta}}$$

- Usual oracle predictive accuracies of $\hat{\boldsymbol{\theta}}$ ($\mathbf{Y}^* = \mathbf{X}\boldsymbol{\theta}^*$, MSE=Mean Squared Error):

$$\Delta\left(\hat{\mathbf{Y}}\right) = \frac{1}{n}\left\|\hat{\mathbf{Y}} - \mathbf{Y}^*\right\|_{2,n}^2 \quad \text{or} \quad \mathrm{MSE}\left(\hat{\mathbf{Y}}\right) = \mathrm{E}\left[\Delta\left(\hat{\mathbf{Y}}\right)\right]$$

Alternative estimate of the OLS

Find an estimator that performs better in terms of predictive accuracy than OLS $\hat{\boldsymbol{\theta}}$

Use a gradient descent algorithm to minimise $g(\boldsymbol{\theta})$ (with fixed step α):

$$\forall k \geq 0, \quad \hat{\boldsymbol{\theta}}^{(k+1)} = \hat{\boldsymbol{\theta}}^{(k)} - \alpha \nabla g(\hat{\boldsymbol{\theta}}^{(k)})$$

- New parameter estimate (this one obtained at iteration k):

$$\hat{\boldsymbol{\theta}}^{(k)} = \left(\mathbf{I}_d - \left(\mathbf{I}_d - \frac{\alpha}{n}\mathbf{X}'\mathbf{X}\right)^k\right)\hat{\boldsymbol{\theta}} + \left(\mathbf{I}_d - \frac{\alpha}{n}\mathbf{X}'\mathbf{X}\right)^k \boldsymbol{\theta}^{(0)} \qquad \left(\overset{k\to\infty}{\longrightarrow} \hat{\boldsymbol{\theta}}\right)$$

- New predictive estimate (this one obtained at iteration k):

$$\hat{\mathbf{Y}}^{(k)} = \mathbf{X}\hat{\boldsymbol{\theta}}^{(k)} \qquad \left(\overset{k\to\infty}{\longrightarrow} \hat{\mathbf{Y}}\right)$$

Expected predictive gain of the new estimate

Stopping at $k < \infty$ can be better than the OLS ($k = \infty$)!

- Result on MSE:

$$\overline{k} = \underset{k \in \mathbb{N}}{\mathrm{argmin}} \left\{ \mathrm{MSE}\left(\hat{\mathbf{Y}}^{(k)}\right) \right\} \quad \Rightarrow \quad \mathrm{MSE}\left(\hat{\mathbf{Y}}^{(\overline{k})}\right) < \mathrm{MSE}\left(\hat{\mathbf{Y}}\right)$$

- Result on Δ (holds with high probability):

$$k^* = \underset{k \in \mathbb{N}}{\mathrm{argmin}} \left\{ \Delta\left(\hat{\mathbf{Y}}^{(k)}\right) \right\} \quad \Rightarrow \quad \Delta\left(\hat{\mathbf{Y}}^{(k^*)}\right) < \Delta\left(\hat{\mathbf{Y}}\right)$$

How to estimate the optimal iteration $\overline{k}$ or k^*?

Scope of the current study

This is a toy study

- Since the OLS is available in closed-form, its computational time is the best

But a prospective study

- Allows to mimic algorithm dependent estimates (numerous: closed-form is rare!)
- Allows to understand some fundamental factors acting in the estimate accuracy
- Allows to glimpse expected difficulties for estimating optimal values of k

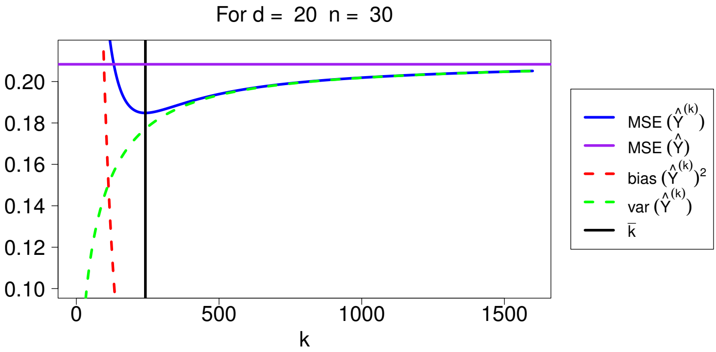
Thus, a step before a future generic method for computational/accuracy trade-off...

Outline

Trade-off bias variance for the MSE

$$\mathrm{MSE}\left(\hat{\mathbf{Y}}^{(k)}\right) = \underbrace{\frac{1}{n}\left\|\mathbf{S}^k\mathbf{P}'\left(\mathbf{Y}^{(0)} - \mathbf{Y}^*\right)\right\|_{2,n}^2}_{\mathrm{bias}\left(\hat{\mathbf{Y}}^{(k)}\right)^2} + \underbrace{\frac{\sigma^2}{n}\mathrm{Tr}\left(\left(\mathbf{I}_n - \mathbf{S}^k\right)^2\right)}_{\mathrm{var}\left(\hat{\mathbf{Y}}^{(k)}\right)}$$

where $\mathbf{K} = \frac{1}{n}\mathbf{X}\mathbf{X}' = \mathbf{P}\boldsymbol{\Lambda}\mathbf{P}'$; $\mathbf{S} = \mathbf{I}_n - \alpha\boldsymbol{\Lambda}$; $\alpha = 0.01 \in \left]0, \frac{1}{\hat{\lambda}_1}\right[$; $\hat{\lambda}_1 = \|\mathbf{K}\|_2$



Something more on optimal values of k

There exists $M_1,\ M_2,\ M_3,\ M_4 > 0$ such as, with high probability, for large n,

$$M_1 + M_2 \log(n) \leq k^* \leq M_3 + M_4 \log(n).$$

- Thus it suggests to perform "few" iterations for small samples sizes
- Somewhat consistent with the fact that the OLS ($k = \infty$) is a "large n" estimate
- But even for large n values, k^* has not to be too high
- And if we perform too many iterations, we have the following variance effect:

$$\forall k \in \mathbb{N}, \quad \mathrm{MSE}\left(\hat{\mathbf{Y}}^{(k)}\right) \geq \frac{\sigma^2}{4n} \sum_{j=1}^{d} \min\left\{1, \left(k\alpha\hat{\lambda}_j\right)^2\right\}$$

Outline

Controlling bias/variance in Δ

Controlling Δ could be possible by (hopefully sharp) inequalities

Highlighting (squared) bias and variance in Δ: $\forall k \geq 0$

$$\Delta\left(\hat{\mathbf{Y}}^{(k)}\right) \leq \underbrace{\frac{2}{n}\left\| E\left[\hat{\mathbf{Y}}^{(k)}\right] - \mathbf{Y}^*\right\|_{2,n}^2}_{B_k^2} + \underbrace{\frac{2}{n}\left\|\hat{\mathbf{Y}}^{(k)} - E\left[\hat{\mathbf{Y}}^{(k)}\right]\right\|_{2,n}^2}_{V_k}$$

We have now to control also B_k^2 and $V_k \ldots$

Controlling the squared bias B_k^2

If $\|\boldsymbol{\theta}^*\|_{2,d} \leq 1$ and $\boldsymbol{\theta}^{(0)} = 0$, $\forall k \in \mathbb{N}$

$$B_k^2 \leq 2\hat{\lambda}_1 \mathrm{e}^{-2k\alpha\hat{\lambda}_d} := B_k^{2,\mathrm{sup}}$$

This upper bound seems to be sharp enough to capture the exponential algorithm dynamic of the (squared) bias observed on the figures!

Controlling the variance V_k

$\exists C_1 > 0$, with probability at least $1 - \mathrm{e}^{-y}$, $\forall k \in \{0 \dots k_{\max}\}$

$$V_k \leq \underbrace{2\mathrm{E}\left[V_k \right]}_{\text{main term}} + C_1 \frac{(y + \log(k_{\max} + 1))}{n}$$

and

$$2\mathrm{E}\left[V_k \right] \leq \frac{4\sigma^2}{n} \sum_{j=1}^{d} \min\left\{1, \left(k\alpha\hat{\lambda}_j\right)^2\right\} := V_k^{\sup}$$

- This upper bound seems to be sharp enough to capture the quadratic then asymptote algorithm dynamic of the variance observed on the figures!
- $k_{\max}$: not dangerous since it corresponds to the maximum iterations that the practitioner can perform in the real world and it is involved only through a logarithm scale

Stopping rule to estimate k^*

From previous results, we have with probability at least $1 - \mathrm{e}^{-y}$, $\forall k \in \{0 \ldots k_{\max}\}$,

$$\Delta\left(\hat{\mathbf{Y}}^{(k)}\right) \leq B_k^{2,\sup} + 2\mathrm{E}\left[V_k \right] + C_1 \frac{(y + \log(k_{\max} + 1))}{n}.$$

From it, we propose the two following estimates for k^*:

$$\hat{k}_1 = \min\left\{k \in \mathbb{N} : B_{k+1}^{2,\sup} + 2\hat{\mathrm{E}}\left[V_{k+1} \right] > B_k^{2,\sup} + 2\hat{\mathrm{E}}\left[V_k \right]\right\}$$

$$\hat{k}_2 = \min\left\{k \in \mathbb{N} : B_{k+1}^{2,\sup} + \hat{\mathrm{E}}\left[V_{k+1} \right] > B_k^{2,\sup} + \hat{\mathrm{E}}\left[V_k \right]\right\}$$

where $\hat{\mathrm{E}}\left[V_k \right] = \frac{2\hat{\sigma}^2}{n} \sum_{j=1}^{d} \left(1 - \left(1 - \alpha\hat{\lambda}_j\right)^k\right)^2$

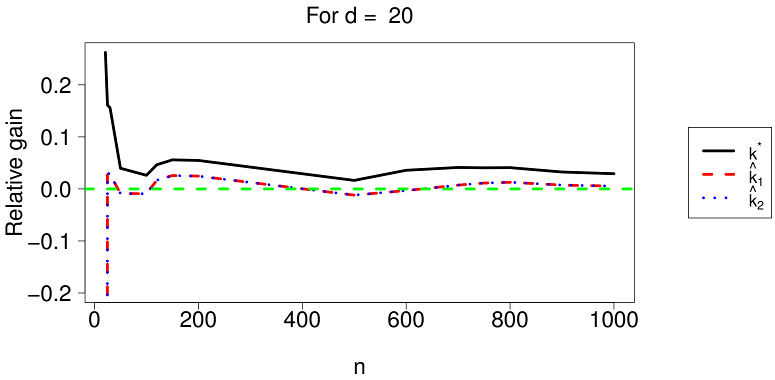
Note: not completely satisfactory since estimate $\hat{\sigma}^2$ is required. . .

Outline

Definition of the relative gain

$$\mathrm{GainRel}\left(\hat{\mathbf{Y}}^{(\hat{k})}\right) = \frac{\mathrm{MSE}\left(\hat{\mathbf{Y}}\right) - \mathrm{MSE}\left(\hat{\mathbf{Y}}^{(\hat{k})}\right)}{\mathrm{MSE}\left(\hat{\mathbf{Y}}\right)}.$$

Relative gain as a function of n for $d = 20$



- Estimates $\hat{k}_1$ and $\hat{k}_2$ with confounded behaviour
- Strong correlation with the behaviour of k^*
- Potential gain higher for small n but not too small for (quite) large n
- $n = 21$: unexpected problem for $\hat{k}_1$ and $\hat{k}_2$ ($\hat{\sigma}^2$?)
- $n \geq 22$: not completely satisfactory but not so bad for a first attempt. . .

Thank's!